

Nanofluids Change Phase

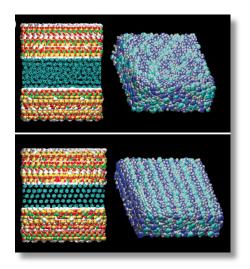
Objective: Atomistic simulations to understand structural and rheological properties of nanoconfined fluids - fluids confined between surfaces separated by just a few nanometers

Implications: Could aid in rational design and control of lubricants for disk drives and microelectromechanical systems (MEMS).

Accomplishments: Convincingly demonstrated that certain nanofluids undergo an abrupt, reversible phase transition into a solid (that would render it useless as a lubricant).

 Showed how increasingly high fidelity molecular simulations provide the ability to understand complex experimental findings, particularly at the nanoscale.

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Results of molecular dynamics simulations run on Franklin showing an organic molecule (blue) confined between two surfaces (red, white, green, and yellow). At a separation of about 41 nanometers (top) the molecule remains fluid-like but at about 30 nanometers (bottom), the molecule undergoes a rapid and abrupt transition to an ordered solid-like structure.



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